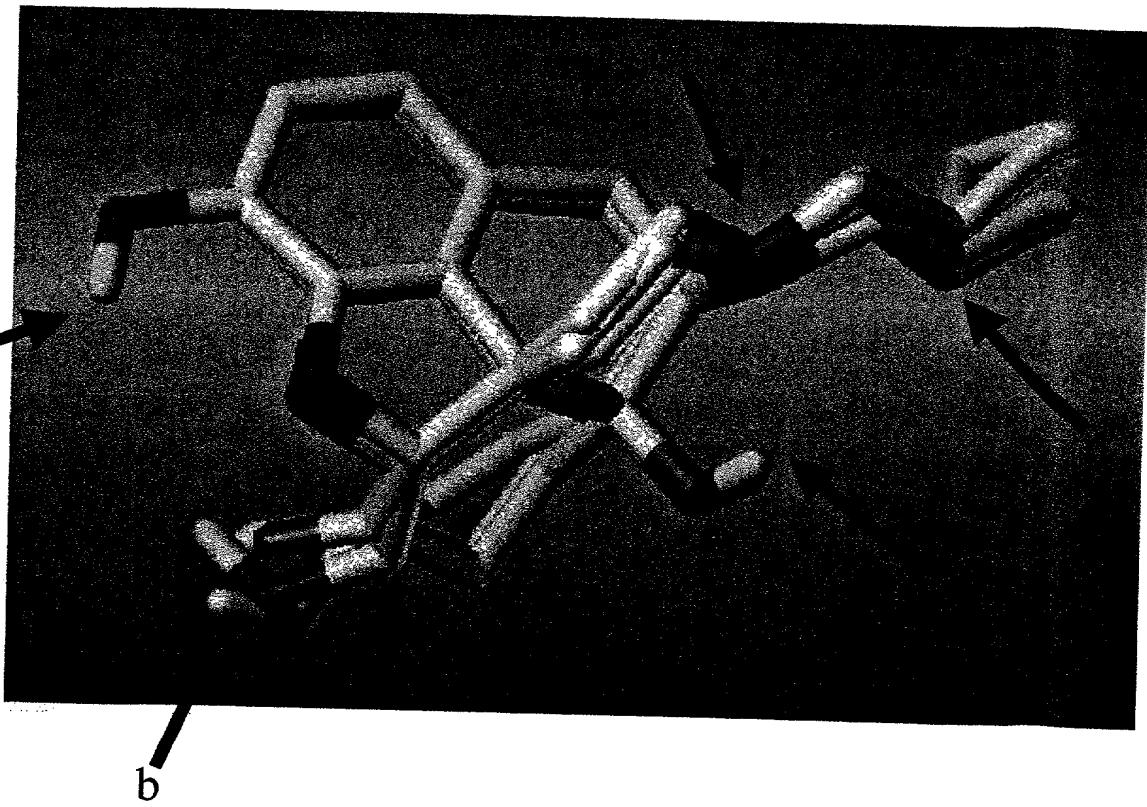
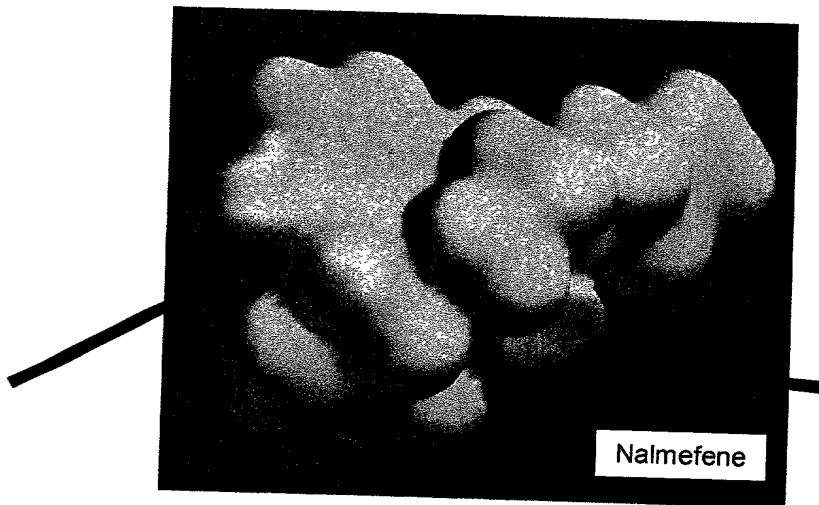
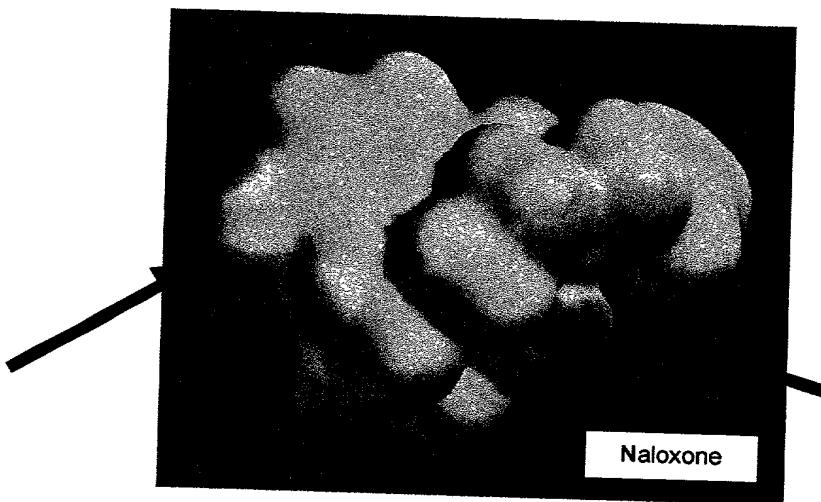
**FIG. 1**



**FIG. 2**



**FIG. 3A**



**FIG. 3B**

## 200 Neighbors

Structure	Cpd ID		MW	Distance	Neighbor
	70413	$C_{19}H_{21}NO_4$	327.384	0.010	Naloxone
	MFCD00133650	$C_{21}H_{25}NO_3$	339.438	0.018	Nalmefene
	349115	$C_{21}H_{27}NO_3$	341.454	0.406	Nalmefene
	BAS 3387173	$C_{18}H_{21}F_3N_2O_3$	370.375	0.510	Naloxone
	BAS 1002455	$C_{16}H_{19}F_3N_2O_3$	344.337	0.519	Naloxone
	BAS 3387155	$C_{17}H_{19}F_3N_2O_3$	356.348	0.524	Naloxone

Fig. 4A

## 200 Neighbors

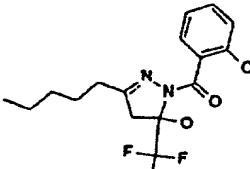
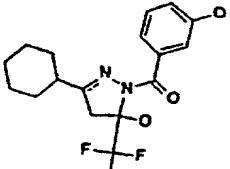
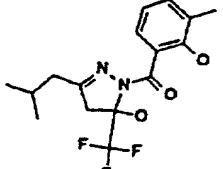
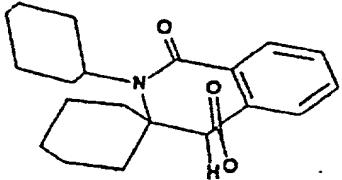
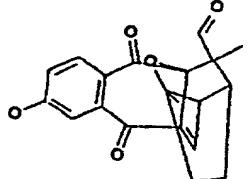
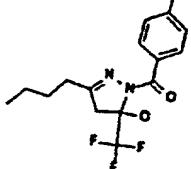
Structure	Cpd ID		MW	Distance	Neighbor
	BAS 1268016	$C_{16}H_{19}F_3N_2O_3$	344.337	0.534	Naloxone
	BAS 3387156	$C_{17}H_{19}F_3N_2O_3$	356.348	0.541	Naloxone
	BAS 3387130	$C_{16}H_{19}F_3N_2O_3$	344.337	0.546	Naloxone
	MFCD01935543	$C_{21}H_{27}NO_3$	341.454	0.551	Naloxone
	688277	$C_{20}H_{18}O_5$	338.363	0.591	6-beta-Naltrixol
	BAS 1002441	$C_{15}H_{17}F_3N_2O_3$	330.310	0.618	Naloxone

Fig. 4B

## 200 Neighbors

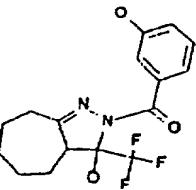
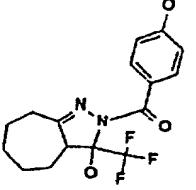
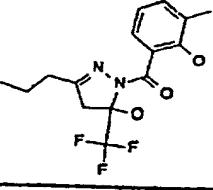
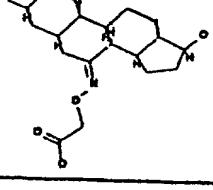
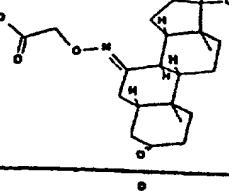
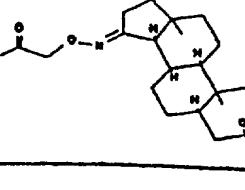
Structure	Cpd ID		MW	Distance	Neighbor
	BAS 3386059	C <sub>16</sub> H <sub>17</sub> F <sub>3</sub> N <sub>2</sub> O <sub>3</sub>	342.321	0.637	Naloxone
	BAS 1003176	C <sub>16</sub> H <sub>17</sub> F <sub>3</sub> N <sub>2</sub> O <sub>3</sub>	342.321	0.637	Naloxone
	BAS 1004848	C <sub>15</sub> H <sub>17</sub> F <sub>3</sub> N <sub>2</sub> O <sub>3</sub>	330.310	0.643	Naloxone
	MFCD00273259	C <sub>21</sub> H <sub>33</sub> NO <sub>5</sub>	379.501	0.644	Nalmefene
	MFCD00273270	C <sub>21</sub> H <sub>31</sub> NO <sub>5</sub>	377.485	0.646	Naloxone
	MFCD00273266	C <sub>21</sub> H <sub>31</sub> NO <sub>5</sub>	377.485	0.648	Naloxone

Fig. 4C

## 200 Neighbors

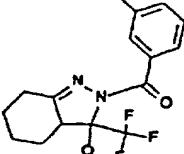
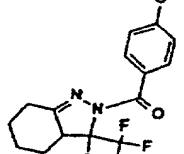
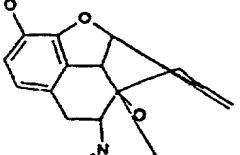
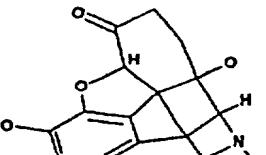
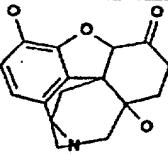
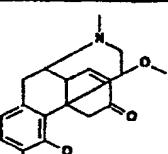
Structure	Cpd ID		MW	Distance	Neighbor
	BAS 3386023	$C_{15}H_{15}F_3N_2O_3$	328.294	0.653	Naloxone
	BAS 2028128	$C_{15}H_{15}F_3N_2O_3$	328.294	0.657	Naloxone
	617005	$C_{18}H_{21}NO_3$	299.373	0.658	6-beta-Naltraxol
	MFCD00079194	$C_{17}H_{19}NO_4$	301.345	0.662	6-beta-Naltraxol
	19045	$C_{17}H_{19}NO_4$	301.345	0.666	6-beta-Naltraxol
	76021	$C_{19}H_{23}NO_4$	329.399	0.673	Nalmefene

Fig. 4D

## 200 Neighbors

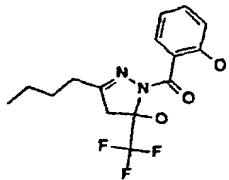
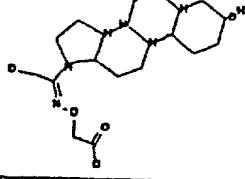
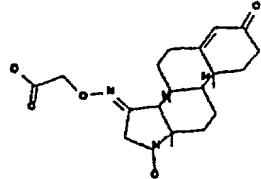
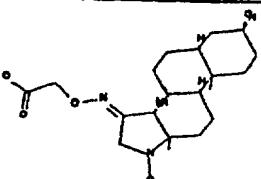
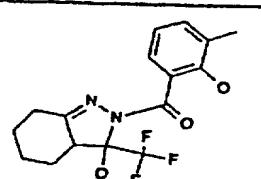
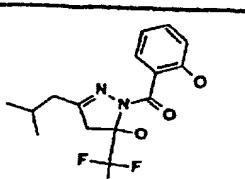
Structure	Cpd ID		MW	Distance	Neighbor
	BAS 1002442	$C_{15}H_{17}F_3N_2O_3$	330.310	0.677	Naloxone
	MFCD00271723	$C_{23}H_{37}NO_5$	407.555	0.682	Naloxone
	MFCD00273273	$C_{21}H_{29}NO_5$	375.469	0.688	Nalmefene
	MFCD00273264	$C_{21}H_{33}NO_5$	379.501	0.697	Nalmefene
	BAS 2026145	$C_{16}H_{17}F_3N_2O_3$	342.321	0.698	Naloxone
	BAS 3387114	$C_{15}H_{17}F_3N_2O_3$	330.310	0.704	Naloxone

Fig. 4E

## 200 Neighbors

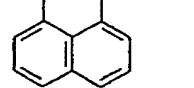
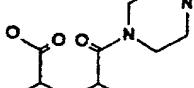
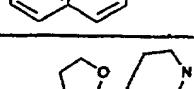
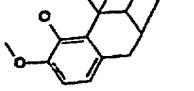
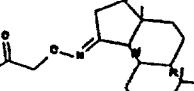
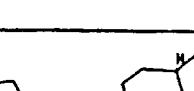
Structure	Cpd ID		MW	Distance	Neighbor
	376679	C <sub>17</sub> H <sub>18</sub> N <sub>2</sub> O <sub>3</sub>	298.345	0.705	Naltrexone
	379963	C <sub>17</sub> H <sub>18</sub> N <sub>2</sub> O <sub>3</sub>	298.345	0.705	Naltrexone
	157870	C <sub>20</sub> H <sub>27</sub> NO <sub>4</sub>	345.442	0.714	Nalmefene
	MFCD00273274	C <sub>21</sub> H <sub>27</sub> NO <sub>5</sub>	373.453	0.720	Naloxone
	MFCD00273260	C <sub>21</sub> H <sub>33</sub> NO <sub>5</sub>	379.501	0.723	Nalmefene
	BAS 1003163	C <sub>16</sub> H <sub>17</sub> F <sub>3</sub> N <sub>2</sub> O <sub>3</sub>	342.321	0.727	Naloxone

Fig. 4F

## 200 Neighbors

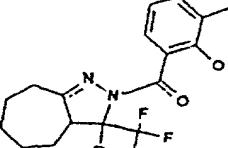
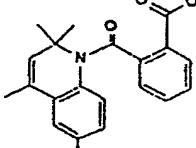
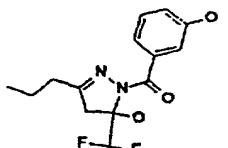
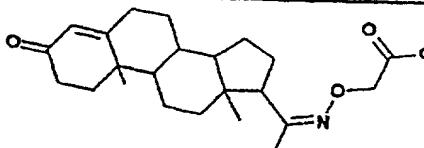
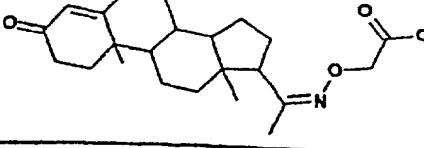
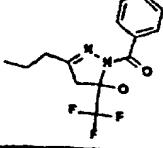
Structure	Cpd ID		MW	Distance	Neighbor
	BAS 1003182	C <sub>17</sub> H <sub>19</sub> F <sub>3</sub> N <sub>2</sub> O <sub>3</sub>	356.348	0.739	Naloxone
	BAS 0510629	C <sub>21</sub> H <sub>21</sub> NO <sub>3</sub>	335.406	0.756	Naloxone
	BAS 1002419	C <sub>14</sub> H <sub>15</sub> F <sub>3</sub> N <sub>2</sub> O <sub>3</sub>	316.282	0.757	Naloxone
	18579	C <sub>23</sub> H <sub>33</sub> NO <sub>4</sub>	387.524	0.760	Nalmefene
	58796	C <sub>23</sub> H <sub>33</sub> NO <sub>4</sub>	387.524	0.760	Nalmefene
	BAS 1004835	C <sub>14</sub> H <sub>15</sub> F <sub>3</sub> N <sub>2</sub> O <sub>3</sub>	316.282	0.763	Naloxone

Fig. 4G

## 200 Neighbors

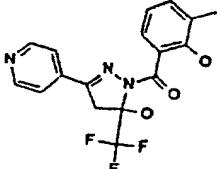
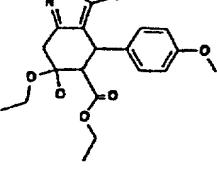
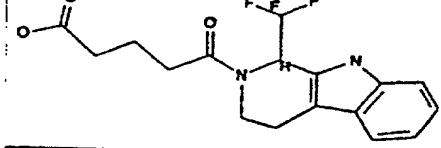
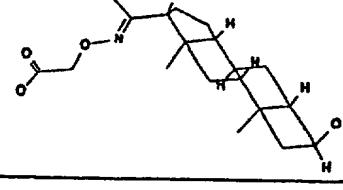
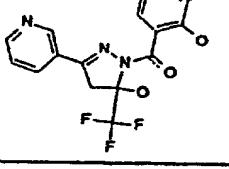
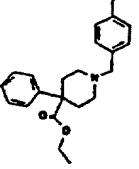
Structure	Cpd ID		MW	Distance	Neighbor
	BAS 2004373	$C_{17}H_{14}F_3N_3O_3$	365.315	0.765	Naloxone
	693856	$C_{19}H_{24}N_2O_6$	376.413	0.768	Nalmefene
	MFCD01764789	$C_{17}H_{17}F_3N_2O_3$	354.332	0.769	Naloxone
	MFCD00271738	$C_{23}H_{37}NO_4$	391.556	0.772	Nalmefene
	BAS 2025996	$C_{17}H_{14}F_3N_3O_3$	365.315	0.774	Naloxone
	BAS 2282169	$C_{22}H_{25}NO_4$	367.449	0.780	Nalmefene

Fig. 4H

## 200 Neighbors

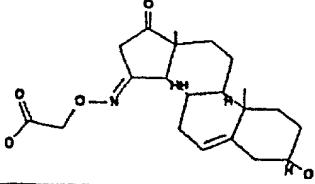
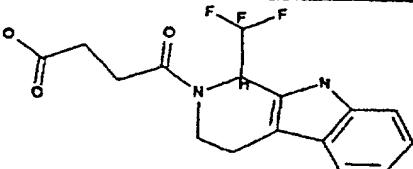
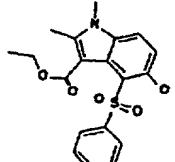
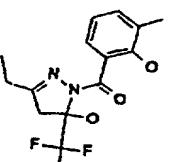
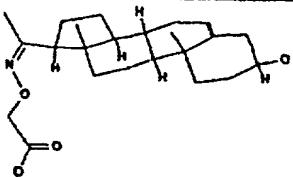
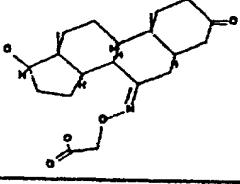
Structure	Cpd ID		MW	Distance	Neighbor
	MFCD00273268	$C_{21}H_{29}NO_5$	375.469	0.789	Naloxone
	MFCD00179880	$C_{16}H_{15}F_3N_2O_3$	340.305	0.800	Naloxone
	BAS 1507170	$C_{19}H_{19}NO_5S$	373.431	0.801	Nalmefene
	BAS 3386088	$C_{14}H_{15}F_3N_2O_3$	316.282	0.802	Naloxone
	MFCD00272082	$C_{23}H_{35}NO_4$	389.540	0.818	Nalmefene
	MFCD00271113	$C_{21}H_{31}NO_5$	377.485	0.829	$\delta$ -beta-Naloxone

Fig. 4I

## 200 Neighbors

Structure	Cpd ID		MW	Distance	Neighbor
	116054	$C_{18}H_{19}N_3O_4$	341.370	0.831	6-beta-Naltrexol
	BAS 1004837	$C_{14}H_{15}F_3N_2O_3$	316.282	0.835	Naloxone
	134536	$C_{19}H_{25}NO_3$	315.416	0.836	6-beta-Naltrexol
	615801	$C_{17}H_{20}N_2O_3$	300.361	0.856	Naltrexone
	404374	$C_{20}H_{27}NO_3$	329.443	0.870	Nalmefene
	MFCD00273318	$C_{23}H_{35}NO_4$	389.540	0.870	Nalmefene

Fig. 4J

## 200 Neighbors

Structure	Cpd ID		MW	Distance	Neighbor
	MFCD00271094	$C_{21}H_{31}NO_4$	361.486	0.877	Nalmefene
	202587	$C_{20}H_{16}O_6$	352.347	0.889	Nalmefene
	693862	$C_{18}H_{20}N_2O_6$	360.370	0.892	Nalmefene
	MFCD00467140	$C_{19}H_{21}NO_4$	327.384	0.905	Nalmefene
	693863	$C_{19}H_{22}N_2O_7$	390.396	0.909	Naltrexone
	MFCD00271196	$C_{21}H_{33}NO_4$	363.501	0.912	Nalmefene

Fig. 4K

## 200 Neighbors

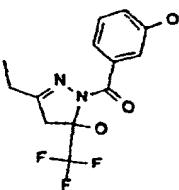
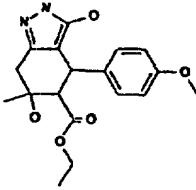
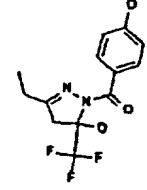
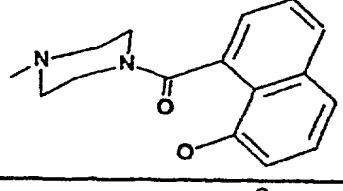
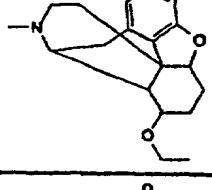
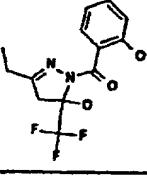
Structure	Cpd ID		MW	Distance	Neighbor
	BAS 3386092	$C_{13}H_{13}F_3N_2O_3$	302.255	0.919	Naloxone
	693855	$C_{18}H_{22}N_2O_5$	346.386	0.923	Nalmefene
	BAS 3386091	$C_{13}H_{13}F_3N_2O_3$	302.255	0.928	Naloxone
	MFCD00665833	$C_{16}H_{18}N_2O_2$	270.334	0.929	Naltrexone
	404368	$C_{19}H_{25}NO_3$	315.416	0.941	$\delta$ -beta-Naltrixol
	BAS 0606820	$C_{13}H_{13}F_3N_2O_4$	318.255	0.948	Naloxone

Fig. 4L

## 200 Neighbors

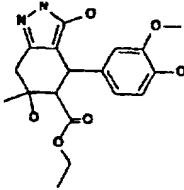
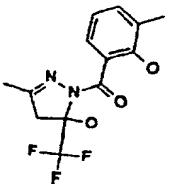
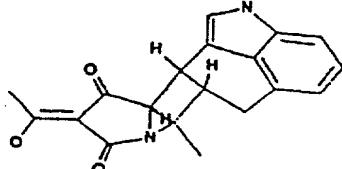
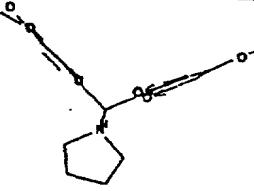
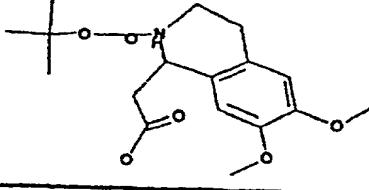
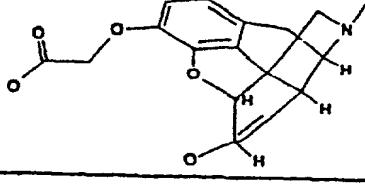
Structure	Cpd ID		MW	Distance	Neighbor
	693859	$C_{18}H_{22}N_2O_6$	362.386	0.949	Naloxone
	BAS 0436353	$C_{13}H_{13}F_3N_2O_3$	302.255	0.965	Naloxone
	MFCD00167445	$C_{20}H_{20}N_2O_3$	336.394	0.968	Naltrexone
	MFCD00667402	$C_{21}H_{25}NO_6$	387.437	0.974	Naloxone
	MFCD02258126	$C_{18}H_{25}NO_6$	351.403	0.977	Naloxone
	MFCD00143186	$C_{19}H_{21}NO_5$	343.383	0.985	Naltrexone

Fig. 4M

## 200 Neighbors

Structure	Cpd ID		MW	Distance	Neighbor
	119887	$C_{21}H_{16}O_5$	348.359	0.993	Naloxone
	404365	$C_{19}H_{25}NO_3$	315.416	1.002	Nalmefene
	MFCD01871411	$C_{21}H_{20}FNO_3$	353.397	1.012	Naloxone
	152720	$C_{18}H_{23}NO_3$	301.389	1.015	$\delta$ -beta-Naltrexol
	117581	$C_{22}H_{19}NO_3$	345.402	1.016	Naloxone
	669466	$C_{15}H_{17}N_3O_4$	303.320	1.017	Naloxone

Fig. 4N

## 200 Neighbors

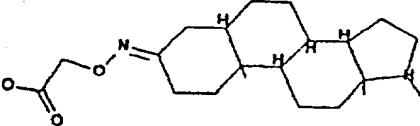
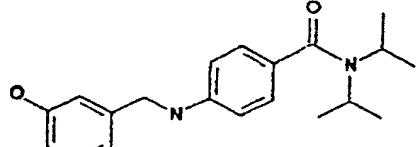
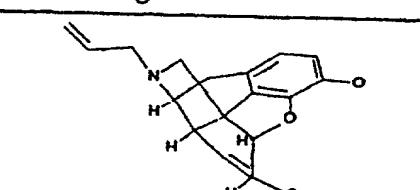
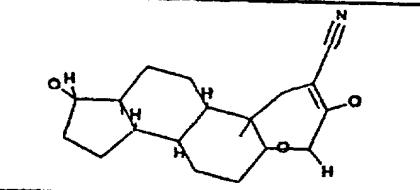
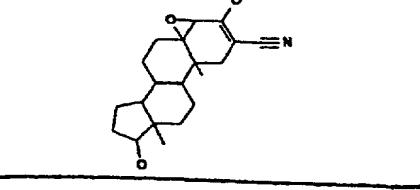
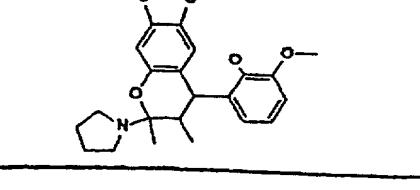
Structure	Cpd ID		MW	Distance	Neighbor
	MFCD00271129	$C_{21}H_{33}NO_4$	363.501	1.029	Naloxone
	689431	$C_{20}H_{26}N_2O_3$	342.442	1.035	6-beta-Naloxone
	MFCD00056772	$C_{19}H_{21}NO_3$	311.384	1.039	Naloxone
	MFCD00199295	$C_{20}H_{27}NO_3$	329.443	1.045	Naloxone
	R191469	$C_{20}H_{27}NO_3$	329.443	1.046	Naloxone
	375504	$C_{23}H_{27}NO_5$	397.475	1.050	Naloxone

Fig. 4O

## 200 Neighbors

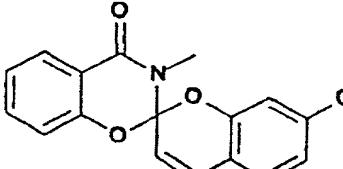
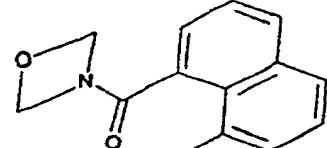
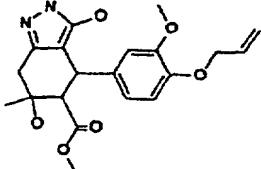
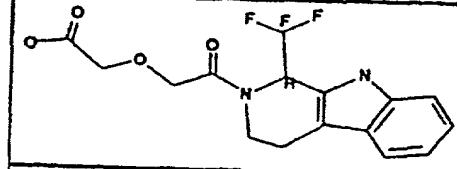
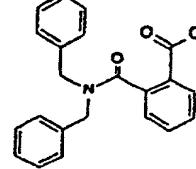
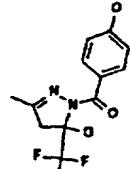
Structure	Cpd ID		MW	Distance	Neighbor
	692397	$C_{17}H_{13}NO_4$	295.297	1.066	Naloxone
	MFCD00433684	$C_{15}H_{15}NO_3$	257.292	1.069	Naloxone
	693860	$C_{20}H_{24}N_2O_6$	388.424	1.071	Nalmefene
	MFCD01764791	$C_{16}H_{15}F_3N_2O_4$	356.304	1.073	Naloxone
	BAS 1519270	$C_{22}H_{19}NO_3$	345.402	1.078	Naloxone
	BAS 3385849	$C_{12}H_{11}F_3N_2O_3$	288.228	1.083	Naloxone

Fig. 4P

## 200 Neighbors

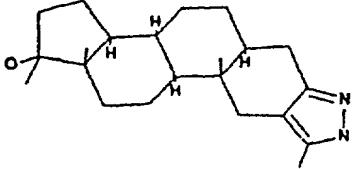
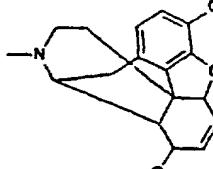
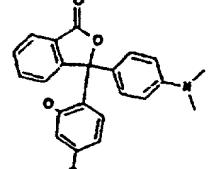
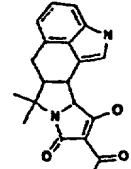
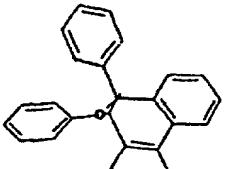
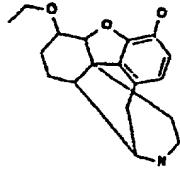
Structure	Cpd ID		MW	Distance	Neighbor
	MFCD00673308	C <sub>21</sub> H <sub>32</sub> N <sub>2</sub> O <sub>2</sub>	344.501	1.087	Naloxone
	404356	C <sub>18</sub> H <sub>21</sub> NO <sub>3</sub>	299.373	1.099	Naloxone
	43938	C <sub>22</sub> H <sub>19</sub> NO <sub>4</sub>	361.401	1.107	Naloxone
	117181	C <sub>20</sub> H <sub>20</sub> N <sub>2</sub> O <sub>3</sub>	336.394	1.109	Naltrexone
	MFCD00094379	C <sub>24</sub> H <sub>22</sub> O <sub>2</sub>	342.442	1.111	Naloxone
	404369	C <sub>19</sub> H <sub>25</sub> NO <sub>3</sub>	315.416	1.111	6-beta-Nalroxol

Fig. 4Q

## 200 Neighbors

Structure	Cpd ID		MW	Distance	Neighbor
	381577	$C_{21}H_{25}NO_7$	403.436	1.111	Naloxone
	S842214	$C_{24}H_{22}O_2$	342.442	1.112	Nalmefene
	134602	$C_{19}H_{21}NO_4$	327.384	1.112	6-beta-Naloxone
	CHS 0316796	$C_{18}H_{25}N_3O_3$	331.418	1.113	Naloxone
	134604	$C_{20}H_{25}NO_4S$	375.491	1.115	Nalmefene
	R171697	$C_{23}H_{27}NO_5$	397.475	1.133	Nalmefene

Fig. 4R

## 200 Neighbors

Structure	Cpd ID		MW	Distance	Neighbor
	MFCD00667401	$C_{23}H_{27}NO_5$	397.475	1.134	Naloxene
	S959863	$C_{18}H_{24}ClNO_3$	337.850	1.137	6-beta-Naloxetanol
	35545	$C_{18}H_{23}NO_3$	301.389	1.137	6-beta-Naloxetone
	134598	$C_{18}H_{23}NO_3$	301.389	1.137	6-alpha-Naloxetone
	S310778	$C_{18}H_{14}O_3$	278.310	1.140	Naloxone
	669800	$C_{17}H_{23}NO_2$	273.378	1.141	Naloxone

Fig. 4S

## 200 Neighbors

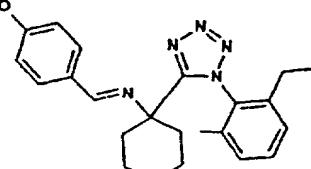
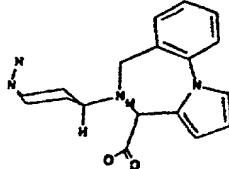
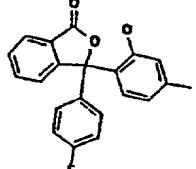
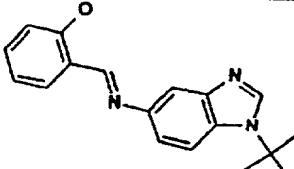
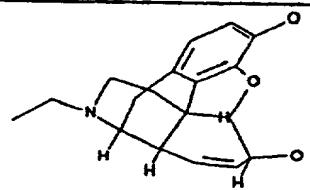
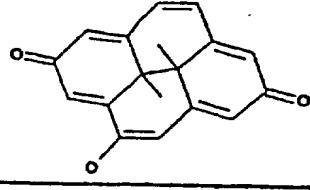
Structure	Cpd ID		MW	Distance	Neighbor
	BAS 0083962	C <sub>23</sub> H <sub>27</sub> N <sub>5</sub> O	389.505	1.141	Naltrexone
	MFCD01765597	C <sub>18</sub> H <sub>21</sub> N <sub>3</sub> O <sub>2</sub>	311.387	1.142	6-beta-Naltrexol
	682334	C <sub>21</sub> H <sub>15</sub> FO <sub>3</sub>	334.350	1.143	Naloxone
	BAS 0631739	C <sub>18</sub> H <sub>19</sub> N <sub>3</sub> O	293.372	1.143	Nalmefene
	MFCD00144882	C <sub>18</sub> H <sub>21</sub> NO <sub>3</sub>	299.373	1.149	6-beta-Naltrexol
	MFCD00229975	C <sub>18</sub> H <sub>14</sub> O <sub>3</sub>	278.310	1.150	Naloxone

Fig. 4T

## 200 Neighbors

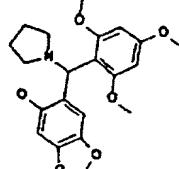
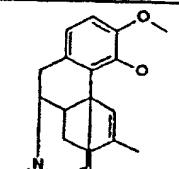
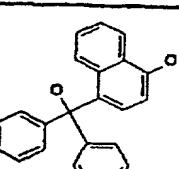
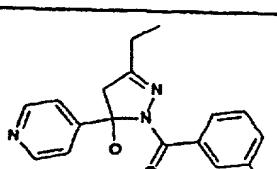
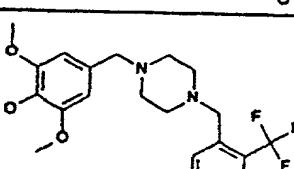
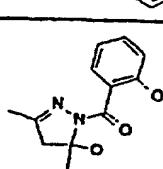
Structure	Cpd ID		MW	Distance	Neighbor
	R171700	$C_{21}H_{25}NO_6$	387.437	1.157	Nalmefene
	134592	$C_{19}H_{23}NO_3$	313.400	1.163	6-beta-Naltrexol
	401210	$C_{23}H_{18}O_2$	326.399	1.166	Nalmefene
	BAS 2026074	$C_{17}H_{17}N_3O_3$	311.343	1.172	Naltrexone
	BAS 3050727	$C_{21}H_{25}F_3N_2O_3$	410.440	1.177	Nalmefene
	BAS 0341630	$C_{12}H_{11}F_3N_2O_3$	288.228	1.185	Naloxone

Fig. 4U

## 200 Neighbors

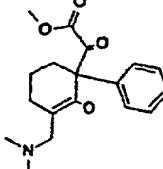
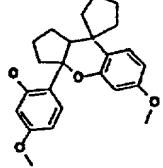
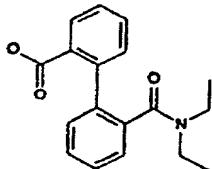
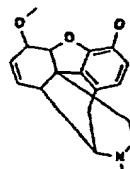
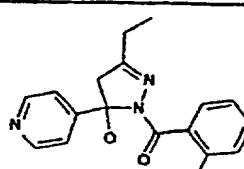
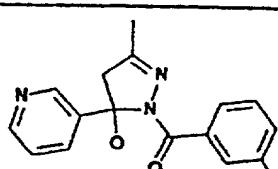
Structure	Cpd ID		MW	Distance	Neighbor
	97817	$C_{18}H_{23}NO_4$	317.388	1.190	Naloxone
	ASN 3185453	$C_{24}H_{28}O_4$	380.488	1.196	Naloxone
	21257	$C_{18}H_{19}NO_3$	297.357	1.196	6-beta-Naltrexol
	134601	$C_{18}H_{21}NO_3$	299.373	1.200	6-beta-Naltrexol
	BAS 2026075	$C_{17}H_{17}N_3O_3$	311.343	1.203	6-beta-Naltrexol
	BAS 1996620	$C_{16}H_{15}N_3O_3$	297.316	1.211	6-beta-Naltrexol

Fig. 4V

## 200 Neighbors

Structure	Cpd ID		MW	Distance	Neighbor
	MFCD01314356	$C_{14}H_{14}F_3N_3O_3$	329.281	1.215	Naloxone
	BAS 2026097	$C_{18}H_{19}N_3O_3$	325.370	1.221	Naltrexone
	BAS 1914007	$C_{21}H_{30}N_2O_3$	358.485	1.221	Naloxone
	CHS 0003221	$C_{16}H_{21}NO_3$	275.351	1.227	Naloxone
	667256	$C_{20}H_{12}O_5$	332.316	1.227	Naloxone
	37625	$C_{25}H_{20}O_2$	352.437	1.235	Nalmefene

Fig. 4W

## 200 Neighbors

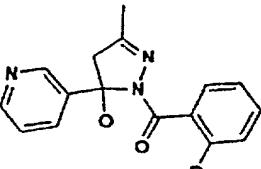
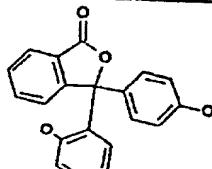
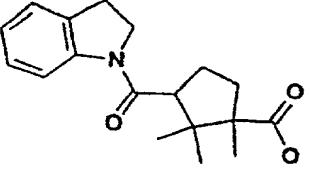
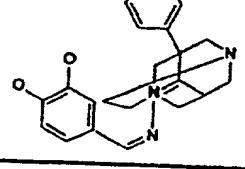
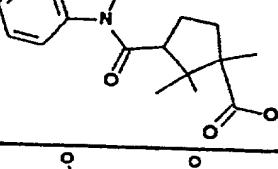
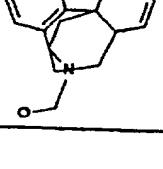
Structure	Cpd ID		MW	Distance	Neighbor
	BAS 1003093	C <sub>16</sub> H <sub>15</sub> N <sub>3</sub> O <sub>3</sub>	297.316	1.236	6-beta-Naloxetoxol
	16468	C <sub>20</sub> H <sub>14</sub> O <sub>4</sub>	318.332	1.238	Naloxone
	CHS 0227049	C <sub>18</sub> H <sub>23</sub> NO <sub>3</sub>	301.389	1.241	Naloxone
	BAS 0315050	C <sub>22</sub> H <sub>24</sub> N <sub>4</sub> O <sub>2</sub>	376.462	1.241	Nalmefene
	BAS 1289763	C <sub>18</sub> H <sub>23</sub> NO <sub>3</sub>	301.389	1.242	Naloxone
	349127	C <sub>17</sub> H <sub>19</sub> NO <sub>4</sub>	301.345	1.243	Naloxone

Fig. 4X

## 200 Neighbors

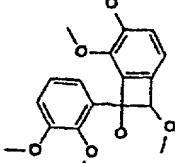
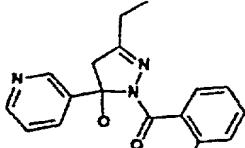
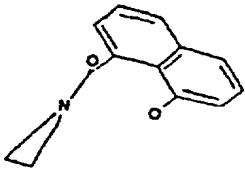
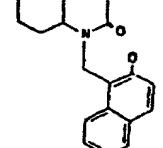
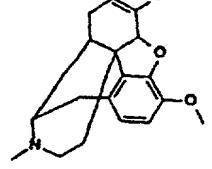
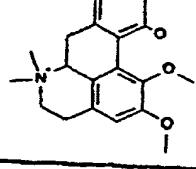
Structure	Cpd ID		MW	Distance	Neighbor
	635928	$C_{18}H_{20}O_6$	332.356	1.250	Naloxene
	BAS 2377555	$C_{17}H_{17}N_3O_3$	311.343	1.251	6-beta-Naltrexol
	MFCD00665835	$C_{15}H_{15}NO_2$	241.292	1.251	Naltrexone
	47931	$C_{19}H_{23}NO_2$	297.401	1.255	6-beta-Naltrexol
	76435	$C_{18}H_{21}NO_3$	299.373	1.257	Naloxene
	90558	$C_{21}H_{26}NO_4$	356.446	1.258	Naloxone

Fig. 4Y

## 200 Neighbors

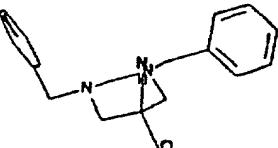
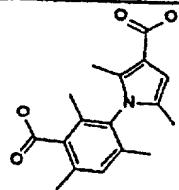
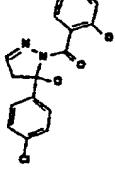
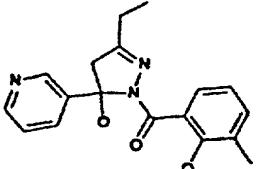
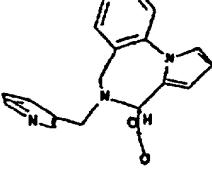
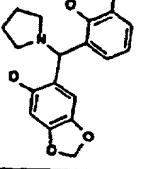
Structure	Cpd ID		MW	Distance	Neighbor
	MFCD00206273	$C_{20}H_{21}N_3O_2$	335.409	1.261	Naloxone
	159208	$C_{17}H_{19}NO_4$	301.345	1.267	Nalmefene
	BAS 0341580	$C_{16}H_{13}ClN_2O_3$	316.747	1.267	Naltrexone
	BAS 2377575	$C_{18}H_{19}N_3O_3$	325.370	1.268	Naltrexone
	MFCD01765638	$C_{19}H_{17}N_3O_2$	319.366	1.268	Nalmefene
	R171484	$C_{20}H_{23}NO_5$	357.410	1.268	Nalmefene

Fig. 4Z

## 200 Neighbors

Structure	Cpd ID		MW	Distance	Neighbor
	700350	$C_{15}H_{23}N_5O_2$	305.383	1.272	Naloxone
	16907	$C_{20}H_{15}NO_4$	333.347	1.274	Nalmefene
	R170623	$C_{21}H_{25}NO_3$	371.437	1.275	Nalmefene
	S98907	$C_{20}H_{14}O_4$	318.332	1.278	Naloxone
	10464	$C_{20}H_{14}O_4$	318.332	1.278	Naloxone
	215214	$C_{20}H_{14}O_4$	318.332	1.278	Naloxone

Fig. 4AA

## 200 Neighbors

Structure	Cpd ID		MW	Distance	Neighbor
	R171425	$C_{20}H_{23}NO_5$	357.410	1.280	Naloxene
	MFCD00153032	$C_{17}H_{19}NO_3$	285.346	1.283	$\delta$ -beta-Naloxone
	S196991	$C_{19}H_{19}NO_3$	309.368	1.285	Naltrexone
	R170291	$C_{20}H_{23}NO_8$	373.409	1.286	Naloxone
	682335	$C_{21}H_{15}FO_3$	334.350	1.287	Naloxone
	MFCD00667377	$C_{20}H_{23}NO_5$	357.410	1.289	Naloxene

Fig. 4AB

## 200 Neighbors

Structure	Cpd ID		MW	Distance	Neighbor
	106242	$C_{21}H_{20}N_2O_2$	332.408	1.294	Naloxone
	R170410	$C_{20}H_{23}NO_6$	373.409	1.299	Naloxone
	MFCD00005912	$C_{22}H_{18}O_4$	346.386	1.300	Naloxone
	MFCD01765637	$C_{20}H_{18}N_2O_2$	318.379	1.302	Nalmefene
	376678	$C_{17}H_{20}N_2O_3$	300.361	1.303	Naltrexone
	MFCD01314431	$C_{18}H_{16}F_3N_3O_3$	379.342	1.303	Naloxone

Fig. 4AC

## 200 Neighbors

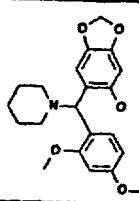
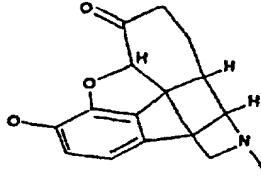
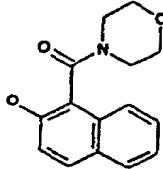
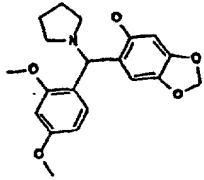
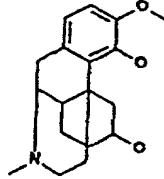
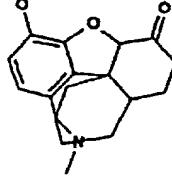
Structure	Cpd ID		MW	Distance	Neighbor
	370278	$C_{21}H_{25}NO_5$	371.437	1.304	Naloxone
	MFCD00242635	$C_{17}H_{19}NO_3$	285.346	1.305	6-beta-Naltrexol
	S602965	$C_{15}H_{15}NO_3$	257.292	1.306	Naltrexone
	370279	$C_{20}H_{23}NO_5$	357.410	1.306	Naloxone
	157877	$C_{18}H_{25}NO_3$	303.405	1.310	Naloxone
	19046	$C_{17}H_{19}NO_3$	285.346	1.310	6-beta-Naltrexol

Fig. 4AD

## 200 Neighbors

Structure	Cpd ID		MW	Distance	Neighbor
	117862	C <sub>17</sub> H <sub>19</sub> NO <sub>3</sub>	285.348	1.310	6-beta-Naltrexol
	MFCD00667305	C <sub>21</sub> H <sub>25</sub> NO <sub>5</sub>	371.437	1.313	Naimefene
	MFCD00667382	C <sub>20</sub> H <sub>23</sub> NO <sub>5</sub>	357.410	1.316	Naimefene
	611276	C <sub>17</sub> H <sub>19</sub> NO <sub>3</sub>	285.346	1.318	6-beta-Naltrexol
	BAS 1099232	C <sub>21</sub> H <sub>22</sub> N <sub>2</sub> O <sub>3</sub>	350.421	1.320	Naltrexone
	BAS 0313319	C <sub>18</sub> H <sub>18</sub> N <sub>2</sub> O <sub>3</sub>	310.356	1.321	6-beta-Naltrexol

Fig. 4AE

## 200 Neighbors

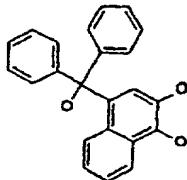
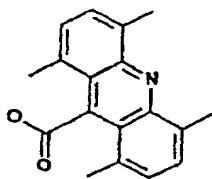
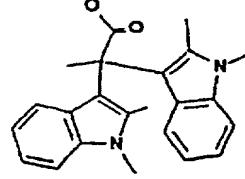
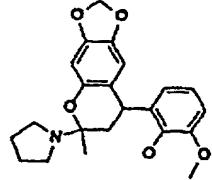
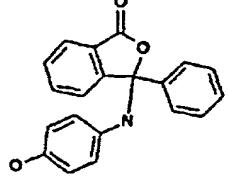
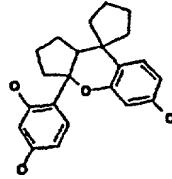
Structure	Cpd ID		MW	Distance	Neighbor
	401211	C <sub>23</sub> H <sub>18</sub> O <sub>3</sub>	342.398	1.325	Naloxone
	409635	C <sub>18</sub> H <sub>17</sub> NO <sub>2</sub>	279.342	1.326	Nalmefene
	106231	C <sub>23</sub> H <sub>24</sub> N <sub>2</sub> O <sub>2</sub>	360.460	1.327	Naloxone
	375505	C <sub>22</sub> H <sub>25</sub> NO <sub>5</sub>	383.448	1.329	Naloxone
	BAS 1053035	C <sub>20</sub> H <sub>15</sub> NO <sub>3</sub>	317.347	1.331	Naloxone
	ASN 3160807	C <sub>22</sub> H <sub>24</sub> O <sub>4</sub>	352.434	1.332	Naloxone

Fig. 4AF

## 200 Neighbors

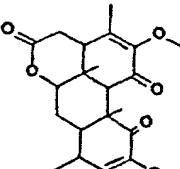
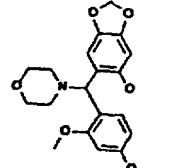
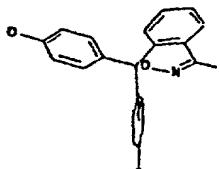
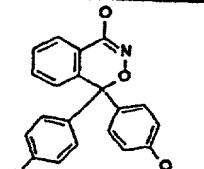
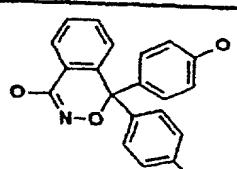
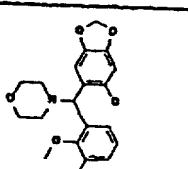
Structure	Cpd ID		MW	Distance	Neighbor
	324633	$C_{21}H_{26}O_6$	374.438	1.333	Naloxone
	370277	$C_{20}H_{23}NO_6$	373.409	1.339	Naloxone
	MFCD00375811	$C_{20}H_{15}NO_4$	333.347	1.343	6-beta-Naltrexol
	BAS 0659522	$C_{20}H_{15}NO_4$	333.347	1.343	6-beta-Naltrexol
	CHS 0305736	$C_{20}H_{15}NO_4$	333.347	1.343	6-beta-Naltrexol
	381576	$C_{20}H_{23}NO_6$	373.409	1.348	Naloxone

Fig. 4AG

## 200 Neighbors

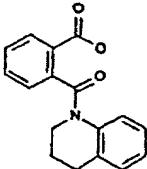
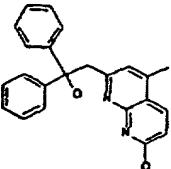
Structure	Cpd ID		MW	Distance	Neighbor
	CHS 0120289	$C_{17}H_{15}NO_3$	281.314	1.348	Naloxone
	351159	$C_{23}H_{20}N_2O_2$	356.428	1.349	Nalmefene

Fig. 4AH